Exotic hadronic states and all-to-all quark propagators

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We discuss methods to obtain accurate hadronic spectra with propagating quarks. Comparing the determination of masses for spin-exotic hybrid mesons with glueball mass determinations, we conclude that quark propagators from all sites to all other sites would enable great improvement in the errors. Such propagators are achievable by using stochastic estimators. We discuss previous attempts and present our method for maximal variance reduction. This is a very promising technique and we illustrate it by obtaining the spectrum of ground state and excited B mesons in the limit where the b quark is static.

1. INTRODUCTION

One of the goals of lattice QCD is to pin down the hadronic spectrum accurately in the quenched approximation and then to explore the shifts as the dynamical quark degrees of freedom are re-introduced. This is particularly relevant to guide experimental searches for glueballs and hybrid mesons. The situation for lattice determination of the spectrum of hybrid mesons, at present, is that the first clear signals have been obtained but much greater precision would be valuable.

It is interesting to contrast this situation with the glueball mass determination for which a precise continuum value has been obtained [1,2] in the quenched approximation. The glueball correlator is measured from all sites on the lattice which gives large statistics even from one gauge configuration. For correlations involving gauge links only, this is very easy to achieve computationally. For correlations involving fermion propagation, the inversion of the fermion matrix from even a single source is computationally expensive. Thus the hybrid correlator has been measured [3,4] from only a single source for each gauge configuration which gives a rather noisy signal. Moreover to construct appropriate non-local sources for hybrid meson studies can also involve extra quark propagator inversions which is costly. The same constraints also apply to a detailed study of the orbital and radial excited hadrons as well.

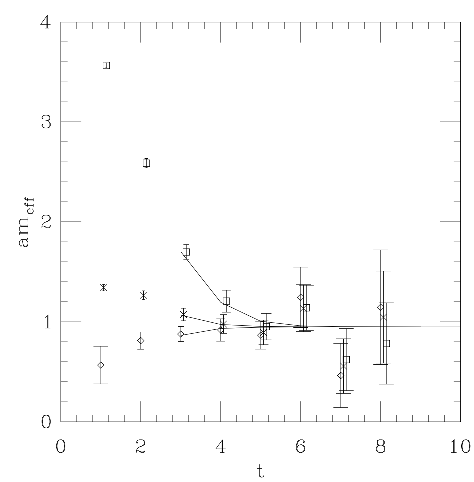

Figure 1. The effective mass of the $J^{PC} = 1^{-+}$ hybrid meson versus t from the UKQCD data [3] with U-shaped source and several different sinks.

The result of the recent UKQCD determination [3] of the spin-exotic $J^{PC} = 1^{-+}$ hybrid meson is shown in Figure 1. This was obtained from 350 propagators from each of two sources separated by a fixed distance and joined by a U-shaped gauge link. By using different operators at the sink, several different correlators were evaluated which allows a separation of ground state and excited states of the required quantum num-

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bers. The study with a clover-Wilson fermion action using $C_{SW} = 1.4785$ at $\beta = 6.0$ and a hopping parameter corresponding to a quark mass close to strange, gave a hybrid meson mass of 2.0(0.2) GeV for the $\bar{s}s$ state. The results for other exotic spin-parity hybrid mesons are consistent with being heavier than this 1^{-+} state.

As already indicated, a more precise determination of these spectra would be valuable. With this in mind, we now discuss the feasibility of evaluating all-to-all hadronic correlators. As an illustration of the potency of this approach, we will present a preliminary study of the spectrum of excited $\bar{b}q$ mesons. Here spin-exotic hybrid mesons cannot be identified because charge conjugation C is not a good quantum number. Nevertheless, lattice studies can guide experimental searches in this area where few experimental results are available.

2. STOCHASTIC PROPAGATORS

The conventional approach to quark propagation in a gauge background field (this discussion applies equally to the quenched case and to full QCD with dynamical quarks) is to solve the lattice Dirac equation $Q\psi = \delta$ iteratively from a single source to determine a propagator G satisfying $QG = 1$. This problem is equivalent to that of the inversion of a sparse matrix since Q has only local and nearest neighbour contributions – this inversion is solved by iteration which is computationally expensive. For a local source at x, the propagator $G(y, x)$ contains information about the quark propagation from this source to all lattice sites y. For the Wilson-Dirac discretisation (this includes the SW-clover case) then $Q(x, y) = \gamma_5 Q(y, x)^* \gamma_5$ and hence the propagation from all sites to the source is also obtained. Thus in the usual approach, only propagators to or from $x = (0, 0, 0, 0)$ are determined. This limits the correlations that can be constructed to explore hadronic spectra and matrix elements and can cause large statistical errors and large correlations among different t values since so few samples of the correlation are evaluated for each gauge configuration.

In the case of a meson with one static quark and one propagating light quark, then only the elements of G with the same spatial component $\mathbf{x} = \mathbf{y}$ will be used in such correlations and two such numbers (from positive and negative time directions) per gauge configuration will be available for use to study the correlation versus time t. Thus only a very small part of the information obtained labouriously by inverting Q to obtain G is used in this extreme case. An attractive alternative is to obtain the propagator from many different sites. The default way to achieve this is just to repeat the inversion for sources at different positions. This is computationally demanding and, if the propagators were to be stored, would involve prodigious storage requirements for all-to-all propagators.

An alternative route is to accept stochastic estimators of the propagators. Since the fermion matrix inversion is conducted in a gauge field sample, it is not necessary to determine the propagator G to 10 digit accuracy as is usually done. Indeed, varying the elements of the propagator randomly by a few percent makes little change to the hadronic correlators obtained. The problem is to achieve this stochastic sampling in an unbiased way. Just stopping the inversion algorithm at relative accuracy of 1% introduces bias. One acceptable approach is to use a pseudo-fermion method with scalar fields interacting via the fermion matrix. This amounts to obtaining a stochastic estimate of the inverse of a matrix M by use of the gaussian Monte Carlo process:

$$Z = \int D\phi \; e^{-\frac{1}{2}\phi^* M \phi} \qquad (1)$$

with $M^{-1}_{ji} = <\phi^*_i \phi_j>$. This approach requires a positive definite matrix M which can be arranged by taking $M = Q^\dagger Q$ where Q is the Wilson-Dirac fermion matrix. Then M will be sparse (it has at most next to nearest neighbour terms) and the Monte Carlo process can be simulated efficiently. Taking $\alpha = 1, \ldots N$ samples of the scalar fields ϕ^α_i yields stochastic estimates of the inverse of M. Thence the propagator Q^{-1} can be recovered from these samples since $G_{ji} = Q^{-1}_{ji} = <(Q_{ik}\phi_k)^* \phi_j>$.

The stochastic evaluation of propagators has the advantage that the number of correlations

measured increases hugely - by L^3T for a lattice of spatial size L and time length T. This is compensated by the increase in error from the stochastic (rather than exact) propagators used. The statistical error is easily estimated since each scalar field ϕ_i has a variance of order 1 (here we normalise the Wilson-Dirac matrix as $Q = 1 - KD$ with hopping parameter K). Thus for N samples each propagator will have errors of order $N^{-1/2}$. This will result in a statistical error on hadron correlations which is independent of time separation t. So for small t one will have small relative errors while at larger t the relative error will be huge since the signal is so small. Since hadron correlators at reasonably large t values are needed to separate out ground states and excited states, a way to reduce these statistical errors is essential.

One suggestion [5] is to use a local multi-hit variance reduction for the ϕ fields. This is equivalent to taking an improved estimator for the ϕ field which is the average over many Monte Carlo updates of that field with its neighbours held fixed. This is very easy to implement and provides a significant error reduction. This approach has been used for B-meson physics successfully [5]. Such a variance reduction is a welcome amelioration but still does not give an absolute error decreasing with t. This very attractive goal can, however, be achieved and here we present our proposals.

Imagine that instead of a multi-hit update of one site in the presence of its neighbours held fixed, one considered the updating of a fixed region P. Let the scalar fields within P be labelled ϕ and those on the boundary of P be labelled s. Then the required improved estimate of ϕ with s held fixed is given by

$$v_i = \frac{1}{\mathcal{Z}} \int D\phi \, \phi_i e^{-\frac{1}{2}(\phi_j^* \hat{M}_{jk} \phi_k + \phi_j^* \tilde{M}_{jk} s_k + h.c.)} \qquad (2)$$

where we have distinguished the elements of M connecting the set of ϕ fields inside P to themselves ($\hat{M}$) and those connecting them to the boundary ($\tilde{M}$). The integral over ϕ is gaussian and we obtain:

$$v_i = -\hat{M}_{ij}^{-1} \tilde{M}_{jk} s_k \qquad (3)$$

This can be visualised as the propagator $\hat{M}^{-1}$ in region P from source $\tilde{M}s$ at the boundary to site i. We will call v the maximally variance reduced stochastic estimator. If site i lies a minimum of d links from the nearest boundary point, then we would expect v_i to decrease in magnitude as d increases. In the lowest order hopping parameter expansion this behaviour will be as K^d. Since the variance of s will remain of order one, this implies that the variance of v will be maximally reduced by taking a partition P which has a boundary as far as possible from the point i. However, we must remember that this variance reduction formula applies if just *one* ϕ field within P is to have its variance reduced. To evaluate a variance reduced propagator one must choose two disjoint regions P and R and solve for the variance reduced fields v_i and w_j in P and R respectively. Then we will have $G_{ji} = < v_i^* w_j >$ with no bias. Thus the rules of operation are to take regions P and R around points i and j such that the boundaries of P and R are as far from these points as possible.

One geometry which allows this is to take P as the time slices $0 < t < T/2$ and R as the time slices $T/2 < t < T$. The boundary sources S are then the time slices at $t = 0$ and $T/2$. Then propagators between P and R (also between P and S and between R and S) can be evaluated with maximal variance reduction. This is not all-to-all just most-to-most, although by using in turn several different choices of partitioning into P and R, all-to-all can be obtained. We have achieved the goal of stochastic propagators from most sites to most sites but at what computational cost? Each variance reduction operation corresponds to a sparse matrix inversion with a source $\tilde{M}s$ (where s are the stochastic samples of ϕ on the source planes at $t = 0$ and $T/2$) in a region less than half the lattice size. N=12 samples of v and w can be obtained for a computational effort equivalent to one usual inversion of M for all 12 colour-spin components at one source. This increases by a factor of 2 or so the computation of evaluating by Monte Carlo the stochastic fields in the first place. This is more than balanced by the huge reduction in error as we shall see.

Since this procedure is conceptually a triply nested Monte Carlo, we summarise the steps

needed.

- Create gauge configurations g.
- In g, create sample scalar fields for all x and colour-spin components by Monte Carlo using equation 1: $\phi^\alpha(g)$.
- Using the scalar field as a source on time-planes at $t = 0$ and $T/2$, solve iteratively using equation 3 for the improved estimators $v^\alpha(g)$ and $w^\alpha(g)$.
- then $G_{ji} = \sum_g \sum_\alpha (Q_{ik} v_k^\alpha(g))^* w_j^\alpha(g)$.

This procedure will certainly provide maximally variance reduced stochastic estimators of propagators. The number of the stochastic samples N of the scalar field should be chosen so that the resulting error on the quantity of interest from one gauge configuration is small enough but not so small that it is less than the intrinsic variation from one gauge configuration to another. We explore first the case of the B meson using a static approximation for the heavy quark. This is a very favourable case for stochastic inversion since there is a large increase in statistics (through using all space points as sources) and the hadronic correlation of interest is proportional to the light quark propagator so the choice of N is not critical. Our choice of partitions P and R is also seen to be appropriate because propagators are only needed in the time direction for which the variance reduction will have maximal effect.

3. B SPECTROSCOPY

We consider a small lattice (8^3 16) at $\beta = 5.74$ with Wilson fermions of hopping parameter $K = 0.156$. This choice was motivated by pre-existing studies [6]. As a first example we evaluated the B meson correlator at time separation t using local hadronic operators at source and sink. Then we compared conventional inversion with various implementations of stochastic inversion. Sample results are shown in Table 1 where the comparison has been made for equal disk storage of propagators or scalars. We chose $N = 25$ samples to evaluate the stochastic estimates of the propagators. In the maximally reduced variance method,

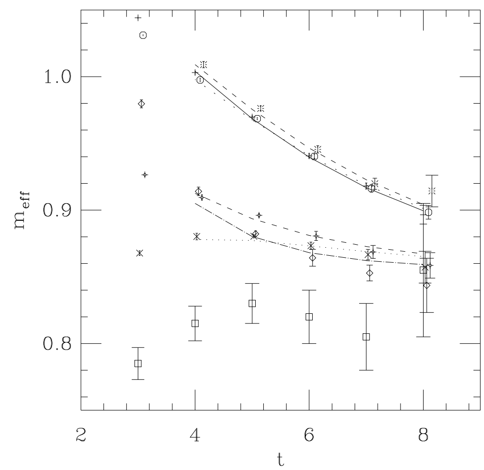

Figure 2. The B meson effective mass versus t from our data with different combinations of local, fuzzed and $\gamma_i D_i$ sources and sinks together with a three exponential fit. Also shown (squares) are the Wuppertal data [6] for smeared source and local sink from 170 propagators.

v_i and w_j were chosen symmetrically either side of the source time planes.

The maximal variance reduction gives a factor of 7 improvement in error compared to other methods for only an overall computational increase of a factor of 4. This is equivalent to a net gain of a factor of 12 in computing time for a similar result. Moreover, the stochastic method allows correlations involving different sources (smeared, fuzzed, etc) to be constructed at little extra cost. This can be seen in Figure 2 which shows the effective mass plots for some of these correlators – these results come from stochastic evaluation from 20480 sources – as described in Table 1. The results [6] from conventional inversions (with 170 sources) are seen to be significantly less precise than those obtained here.

Also illustrated is a three state fit to our hadronic correlations which yields $ma = 0.855(6)$ for the ground state and $m'a = 1.233(15)$ for the first excited state of the same quantum numbers, where the errors quoted are statistical only.

Table 1
B meson correlators at $t = 7$.

Method	$C(7) \times 10^7$	Data Set	CPU
MR inversion	3712(147)	propagators from 4 sources for 10 gauge fields	1
Stochastic inversion		25 samples of ϕ	
Basic	2754(926)	for 20 gauge fields	2
Local multihit	3418(410)		2
Maximal variance reduction	3761(21)		4

We have also extracted the correlations corresponding to the L-excited states (P and D-wave). Of particular interest is the splitting of the P wave level into two energy values in the static heavy quark limit, corresponding to $J^P = 0^+,\ 2^+$ mesons. Our preliminary results are $ma = 1.35(5)$ and $1.24(4)$ respectively, where the errors are purely statistical. Note that, if the level ordering indicated by these preliminary results should be substantiated, this is a first indication of a meson system for which the 2^+ state is lighter than the 0^+. This is not unexpected in potential based models since the relevant spin-orbit splitting has this sign at large distance [8,9]. Further work using larger lattices, several lattice spacings and several hopping parameters is under way to explore this further.

4. HADRONIC OBSERVABLES

For observables with more than one light quark propagator, it is possible to use the stochastic method, but some care is needed. One way to grasp the subtlety is to imagine that there are two quarks with different flavours and to split the sum over samples $\alpha = 1, \dots N$ into subsets for each flavour. Provided these two subsets are independent, then propagators of each flavour are obtained without bias. In practice, provided the stochastic estimators ϕ^α are independent of α, then a sum over $\alpha,\ \beta = 1, \dots N$ with $\alpha \neq \beta$ gives the required information. This illustrates that the number of samples is effectively N^2 for mesons and N^3 for baryons. Indeed we have observed that the error from the stochastic sampling reduces as $1/N$ for correlators involving two light quarks in the region of small N. For large N values, there will be no advantage in reducing the error from one gauge sample to below the intrinsic variation between gauge samples.

We discuss briefly the potential advantages of using stochastic propagators for different hadronic observables. As we have shown above, for heavy quarks in the static limit, light quark propagators are needed in the time direction and these are efficiently produced by the stochastic method with maximal variance reduction. Thus other static observables such as Λ_b and the matrix element B_B are efficiently evaluated.

For mesons made of light quarks, it is necessary to project the correlations into a specific momentum state. This implies a sum of correlations over the whole spatial volume at that time. Even though the signal will be localised at small difference between spatial coordinates of source and sink, in this sum the noise will come from all spatial sites. Another way to see this is that the propagator for t time steps and x space steps will behave in the lowest order hopping parameter expansion as K^{t+x} whereas the variance reduction we have employed above will reduce the error by K^t only. Thus it appears that stochastic inversion will require a relatively large number of samples N to reduce this noise in the case of the momentum zero hadronic correlation.

One interesting area of application is to disconnected quark diagrams - as needed for η meson studies and glueball mixing. The maximal variance reduction technique does not seem promising since the variance reduced average of ϕ_i^2 will involve $\hat{M}_{ii}^{-1}$ which is not easily obtained computationally (this is after all the origin of the problem here anyway). It is feasible to use a more local region P and this has been studied [7].

5. DISCUSSION

Particularly for dynamical fermion configurations which are computationally expensive to obtain, there is a virtue in measuring the hadronic properties from a gauge configuration as completely as possible. We have presented a method to extract correlators from all sources to all sinks to achieve this. Moreover the storage requirements are not excessive. For the case of correlators involving one static quark, the gain in signal is very significant. For exploration of observables involving more than one source and one sink, such as matrix elements or meson-meson interactions, then our proposal is very promising.

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